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ENTROPY OF LIQUID PSEUDOBINARY ALLOYS

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Abstract

A theory is proposed for the entropy of mixing of compound forming liquid binary alloys on the basis of the hard sphere model, in which formation of "molecules" or "chemical complexes" is assumed. In the theory an atom A, an atom B and a "molecule" $A_{\mu}B_{\nu}$ (μ, ν : integer) are approximated by hard spheres with different diameters and the number of these particles are determined by a kind of equilibrium condition. It is straightforward to obtain, according to Mansoori et al's theory, an expression of the entropy for this ternary mixture of hard spheres. The theory is applied to liquid Li-Pb alloy because this alloy has been extensively studied experimentally and many experimental data are available. There are three parameters in this theory, which are an entropy contribution from the degrees of freedom of a "molecule", the size of a "molecule" and a constant in the equilibrium condition. It is shown that the experimental data for the entropy of mixing can be explained by taking reasonable values for these three parameters. In particular, the negative entropy of mixing near the stoichiometric composition is well reproduced and is attributed to the formation of "molecules". It is also shown that the composition dependence of the electrical resistivity for liquid Li-Pb alloy can be explained qualitatively on the basis of the same model. The peak of the electrical

resistivity may be attributed to strong scattering by the virtual bound states formed in the "molecule" because these "molecules" are not stable in the normal chemical sense. The large negative temperature coefficient may be understood qualitatively within our model from the fact that, as the temperature rises, the stability of "molecules" decreases. From this it follows that the number of "molecules" decreases and therefore the number of conduction electrons increases. The changing sign of the thermoelectric power at the stoichiometric composition may be attributed to the strong energy-dependent scattering due to the virtual bound states of "molecules".

A full report of this work can be found in K. Hoshino and W. H. Young 1980 *J. Phys. F: Metal Phys.* 10.

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